LCA Methodology

Considering Human Toxicity as an Impact Category in Life Cycle Assessment

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Abstract

Characterization of toxic chemicals with relevance to human exposure does normally not belong to Life Cycle Assessments (LCA) and is still a topic of research. The concept of hazard potential classes proposed in this paper is primarily based on threshold limit values that are considered to be a measure of the severity of potential effects. In the absence of threshold limit values the R-phrases of the ordinance of dangerous substances are used. Substances are assigned to five hazard potential classes (A to E). Potentially dangerous chemicals are identified and substances of low toxicological relevance are excluded from further evaluation. The location where a probable exposure might occur (indoor versus outdoor) and inter-media transport of substances is considered. The product comparison is based both on the results of the proposed "semi-quantitative screening method" and on toxicological expert knowledge.

Keywords: Dangerous substances, R-phrases; hazard potential classes, dangerous substances; human exposure, toxic chemicals; indoor exposure; outdoor exposure; semi-quantitative screening method; toxic chemicals, characterization

1 Introduction

There are several approaches to the impact category "human health". One possibility is to use threshold limits as a measure of human toxicity. The "critical volume" method characterizes each emission with the volume of air or water required to dilute the threshold limit set for that emission (BUWAL, 1984; HABERSATTER, 1991). Critical volumes of individual substances can be summated to give a total critical volume. The approach is applied by many LCA practitioners and is incorporated into many databases and software systems.

As a development of the "critical volume" approach, HEIJUNGS et al. (1992) proposed the "provisional method". The human toxicological classification factors for air and water are for example calculated from tolerable concentrations in air (kg/m^3) or acceptable or tolerable daily intake (kg substance per kg body weight) defined by the RIVM or the WHO. The "provisional method" was later replaced by applying the "Uniform System for the Evaluation of Substances" (USES 1.0) to the determination of equivalency factors (GUINÉE et al., 1996a; GUINÉE et al., 1996b). A margin of safety (MOS) is defined as a type of acceptable daily intake (ADI) divided by the predicted daily intake (PDI). The human toxicity potential (HTP) of a substance is calculated by dividing the MOS of the reference substance 1,4-dichlorobenzene by the MOS of the substance. The EU considers the (E)USES system to be the appropriate risk assessment tool for chemicals because it makes allowances for the fate of substances in the environment. The model takes into account degradation, advection and diffusion processes. Exposures can be calculated on a regional scale. Although the future perspectives for (E)USES in LCA are promising, there are some weaknesses:

1. The "unit world" model computes only one concentration value for each compartment, whereas measurements indicate that actual concentrations in the environment may range over several orders of magnitude
2. The general fugacity approach is not appropriate for all kind of substances (e.g., NO_x, CO, particles, metals, substances that dissociate or associate, polar chemicals)
3. The (E)USES model was designed for constant emission flows but the pattern of emission is mostly unknown from the Life Cycle Inventory
4. For the purposes of LCA, the advective flows to unit worlds in the neighbourhood are set equal to zero (that is the residence times in air and waters have been maximized)
5. Additional uncertainty occurs where many of the data are approximated with (worst case) default values or are calculated by QSAR. Approximations are also used for the meteorological conditions and the oral intake parameters
6. There is a lack of toxicity categories. Qualitative risk characterisation for human health is performed for genotoxic, (possibly) carcinogenic or sensitising substances.

Int. J. LCA 3 (2) 80 – 85 (1998)

2 The Concept of Hazard Potential Classes

In this article we suggest a "semi-quantitative screening method" for operating the LCA impact category "human toxicity". The methodology is termed as "semi-quantitative" because it connects quantitative mass loadings per substance (in kg) with qualitative classifications and aspects in the effect and exposure assessment. Examples for qualitative aspects are the use of R-phrases as well as "yes or no decisions" for bioaccumulation or biodegradability.

The proposed system is part of the LCA impact assessment software package ELA (Environmental Loadings Analysis) that was developed by the Fraunhofer Gesellschaft (HERRCHEN et al., 1997a; LEPPER et al., 1997; KELLER et al., 1996; WALZ et al., 1996). The screening method allows a first temporary classification of substances on the basis of data from preceding inventory analyses. The methodology proposed here should overcome some of the obstacles in toxicology assessment:

- It should, if possible, exclude incorrect conclusions caused by too many simplifications.
- It provides a high number of assessable substances by the use of TRGS 905 classifications and R-phrases.
- It distinguishes between different endpoints such as carcinogenicity or skin irritation.
- It distinguishes between different types of emissions (indoor versus outdoor).

Depending on toxicological characteristics as described below, substances are assigned to four preliminary toxicological potential classes (a – d). The potential class is the higher, the lower the corresponding threshold and/or the more serious the effect is (→ *Table 2 and 3, p. 83 and 84*). This means that the different classes partly reflect the potential severity of different effects. The toxicity classification in subcategories was discussed by JOLLIET (1996). Class "a" consists of substances that are of low toxicological relevance for humans. Class "b" or "c" contain substances that may cause adverse effects on the human health in certain circumstances (medium or high toxicity). Class "d" contains chemicals that have been classified as carcinogenic or mutagenic by (inter)national authorities (very high toxicity).

Before the final assignment, it will be checked whether exposure criteria like persistence and accumulation or indoor versus outdoor lead to a more severe allocation. Starting from the preliminary four toxicological potential classes this results in five hazard potential classes HPC_A – HPC_E. According to the expert group of the OECD Hazard Assessment Project (OECD, 1982), the term "hazard" is determined by exposure and noxious effects, both biological and non-biological. An example for the classification of emissions to the different potential classes is presented in LEPPER et al. (1997).

3 Prerequisites for the Evaluation of Emissions

The preliminary condition for the evaluation of emissions within the screening method is the identification of every emitted substance by its CAS-number. Mixtures are separated into their primary constituents that are then separately evaluated. If this is not possible, leading compounds are identified and it is assumed that the total amount emitted is by these compounds.

Usually the amounts of specific substances emitted into air and water are determined during the inventory step. Inventories of some life cycle stages might also provide information as to whether an emission takes place in a closed room or the outdoor environment. This permits assessment of a partial exposure potential.

4 Toxicity Assessment for Airborne and Waterborne Emissions

In a first approximation, occupational threshold limits are considered to give an indication of the severity of potential effects and can be used for a classification within an impact assessment. German MAK-values (maximum workplace concentrations) as well as TLVs from the ACGIH are used. In the absence of these, classifications according to TRGS 905 or otherwise risk phrases (R) of the dangerous substances are used (→ *Table 1*). The R-phrases are grouped into four categories which in a first approximation correspond to the ranges of threshold limit values specified in Table 2 and 3 (*p. 83 and 84*). The use of R-phrases considerably increases the number of assessable substances.

Table 2 and 3 (*p. 83 and 84*) show the classifications and characteristics of substances and preparations in accordance with EG directive 67/548/EEC (inc. 21st amendment) – published under section 4a of the ordinance on dangerous sub-

Table 1: Important EU classification flags based on biological effects and used in Table 2 and 3

May cause cancer by inhalation (R49)	May cause cancer (R45)
May cause mutation in humans (R46)	Possible risk of irreversible effects (R40)
May cause sensitisation by inhalation (R42)	May cause sensitisation by skin contact (R43)
Danger classification very toxic (R26, R27, R28)	Danger classification toxic (R23, R24, R25)
Danger classification harmful (R20, R21, R22)	Corrosive (R34 or R35)
Risk of serious damage to eyes (R41)	Irritating to eyes (R36), the respiratory system (R37), or skin (R38)

stances (GefStoffV) – as well as the substances listed in the TRGS 905 "Index of substances which can cause cancer, genetic changes or limit reproductive capability" (EU, 1996; DFG, 1996; BIA 1996).

For substances that are considered mutagenic (M), carcinogenic (C) or dangerous to human fertility (R_F) or development (R_E) the EU has formulated criteria defining 3 different categories of hazard. The order of risk decreases from category 1 to 3.

Substances showing effects without threshold values, here mutagenicity and carcinogenicity, are classified according to the TRGS 905. Substances suspected of carcinogenic effects (C3; MAK IIIB) are distinguished from substances with known carcinogenic effects (C1 or C2; MAK IIIA1 or IIIA2; Annex I Directive 67/548/EEC: R45, R49). A classification C1 or C2 excludes the derivative of a threshold limit value. Substances with cancer-producing or genotoxic effects (M1, M2, R46) are assigned into the maximum hazard potential class "d".

Two hundred chemicals that occur frequently in the environment or which are assessed in LCAs have already been classified and included into the Fraunhofer procedure for LCA. However, in rare cases it is necessary to adjust the resulting classifications by expert judgement.

In analogy to emissions into the air, toxicity for *waterborne emissions* is evaluated with the aid of acceptable daily intake (ADI) values from the WHO (FAO, 1995) and also with R-phrases (→ *Table 3, p. 84*).

If none of the above limits or classifications are available for a substance, the medium potential class "b" is assigned as default-value.

5 Qualitative Exposure Assessment

The inventory table normally shows the aggregated mass loading per substance without information on time and space. An indirect measure for exposure concentrations are the emitted amounts, which depend on the definition of the so-called functional unit. The larger the variable "functional unit" is, the higher are the emitted quantities. Consequently, the emission by itself is no criterion for the level of possible exposure.

5.1 Emissions into air

Emissions into air lead to a direct exposure by inhalation or dermal contact and, therefore, are of special relevance. The most important aspect for an estimation of exposure is the probability that high concentrations of a substance will occur. Depending on the available data from the preceding inventory a distinction is made between indoor and outdoor emissions (Potting & Hauschild, 1997). The difference is not related to possible effects but to the exposure situation. The same amount of substance emitted in indoor air gives much higher concentrations than if emitted into outdoor air due to the different dilution and is therefore allocated to a higher potential class.

Indoor exposure includes work environment (LCA stage: production) or use of products (LCA stage: application). An example is the application of paints or adhesives indoors. Outdoor exposure includes pollutants caused by traffic, power production, emission via chimneys, etc.

The application of criteria like persistency or bioaccumulation for emissions to air emphasises the possible regional or even global effects of a pollutant. This is more important in the impact category ecotoxicity (Herrchen et al., 1997a), whereas human toxicity is often considered to be a local environmental problem (Saur, 1997). For airborne emissions the effect of persistency (increase of concentration) is at least partly cancelled by the lowering of concentration due to dilution effects.

5.2 Emissions into water

Emissions into water can lead to an (in)direct exposure of the population via drinking water or the food chain. If chemicals do not degrade in water, soil or sediments, plants and animals may take them up. Depending on the ability of the chemical to bioaccumulate, further enrichment via the food chain is possible. In this way environmental chemicals can reach the human body with food or drinking water. In the case of strongly accumulating substances, critical tissue levels may be reached. For example, relatively high concentrations of chlorohydrocarbons in mothers' milk are often observed.

Therefore, for the indirect exposure through environmental chemicals, the classification is based on the substance's inherent properties: toxicity, persistence and bioaccumulation potential. Biodegradable substances do not lead to a relevant human exposure and are excluded from further evaluation of toxic effects.

Degradability can be classified according to the criteria of the EEC directives or the OECD technical guidelines. Bioaccumulation is expressed as the measured biological concentration factor (BCF). According to the EEC directives, the partition coefficient between n-octanol and water (Pow) can be used as a substitute.

6 Exposure and Effect Assessment – Airborne Emissions

Indoor emissions are assigned into the respective next higher potential class compared to outdoor emissions (a → B; d → E, etc.). Substances emitted into the atmosphere remain in their original potential class (a → A; d → D, and so on).

Table 2: Assignment of chemicals into toxicological potential classes and hazard potential classes (HPC) for emissions into air. The hazard potential increases when proceeding from class A to E

Threshold Limit Values (TRGS 900)	Classification according to TRGS 905[a]	Classification according to the Ordinance on Dangerous Substances (GefStoffV)[b]	Toxicological Potential Class	Outdoor Emission HPC_{Air}	Indoor Emission HPC_{Air}
TLV >= 400 mg/m³		R20, R21, R22, R36, R37, R38, R34	a	A	B[c]
TLV >= 5 mg/m³, < 400 mg/m³	R_F3, R_E3	R23, R24, R25, R39/23, R39/24, R39/25, R40/20, R40/21, R40/22, R35, R41, R64, R33, R48/20, R48/21, R48/22, R62, R63; default value	b	B	C
TLV < 5 mg/m³	C3 (MAK: IIIB), M3, R_F1, R_F2, R_E1, R_E2	R26, R27, R28, R39/26, R39/27, R39/28, R42, R43, R48, R48/23, R48/24, R48/25, R40, R60, R61	c	C	D
	C1 or C2 (MAK: IIIA1 or IIIA2), M1, M2	R45, R49, R46	d	D	E

[a] R_F 1,2, or 3: Embryo damaging; R_F 1,2, or 3: Impairment of fertility; M 1,2, or 3: Mutagenicity (EU-commission)
[b] See **Table 1** for details
[c] For TLVs ≥ 400 mg/m³ and < 4000 mg/m³

The hazard potential class E is reserved for indoor emissions of carcinogenic or mutagenic materials. If no distinction between indoor and outdoor- emissions is possible (e.g. open hall in a factory) or no data are available, emissions are treated as emissions into the atmosphere.

7 Exposure and Effect Assessment – Waterborne Emissions

Differences are made between:

1) Toxicity of compounds that are readily biodegraded (exclusion from further evaluation)
2) Toxicity of not readily degradable (persistent or inherently degradable) compounds
3) Toxicity of not readily degradable *and* potential bioaccumulating compounds

Compared to pollutants with property combination 2), pollutants with property combination 3) are allocated to the respective next higher potential class (a → B; d → E, etc.).

8 Inter-Media Transport

For emissions into water also the indirect emissions via the atmosphere must be evaluated. By the computation model MACKEY Level 1 (MACKAY, 1991) the equilibrium distribution between water, soil and air (discharge pattern) is therefore evaluated in a qualitative way. For non biodegradable atmospheric emissions with an equilibrium distribution coefficient > 10% for the media water and/or soil an *indirect* exposure via the food chain may be relevant.

Some waterborne emissions can lead to airborne contamination if the volatility of the substance from aqueous solution is high. This may be the case for non biodegradable emissions with an equilibrium distribution coefficient > 10% for the compartment air (e.g. volatile chlorohydrocarbons). A *direct* exposure via inhalative uptake may thus be possible.

Only indirect emissions to soil via air and water are likely (possible exceptions: sewage sludge or pesticides). To avoid double-allocation, emissions are considered only in the entrance compartments water and air. This means that the emissions are not allocated to the HPCs for air and water according to their percentage amounts calculated. If the calculated equilibrium distribution indicates appreciable transfer between compartments, the computer program marks the respective substance to assess the relevance of an indirect exposure of human beings via food or inhalative uptake. This estimation is performed in the subsequent analysis step of the impact assessment (→ *next section*).

9 Presentation and Analysis of Results

In LCA- impact categories like, e.g. "global warming", "acidification" or "ozone depletion" the actual amounts of emitted substances are multiplied by a so-called characterization (weighing) factor before they are added. The result is the equivalent load or the overall effect score for the respective category:

Equivalent Load = Σ amount of substance i (kg) * characterization factor i

For the impact category "human toxicity" depending on the above described criteria chemicals are first assigned to the

Table 3: Assignment of chemicals into toxicological potential classes and hazard potential classes (HPC) for emissions into waters. The hazard potential increases when proceeding from class A to E

ADI (WHO/FAO)[a]	Classification according to TRGS 905[b]	Classification according to the Ordinance on Dangerous Substances (GefStoffV)[c]	Toxicological potential class	Persistent only[d] HPC_{Water}	Accumulating and persistent HPC_{Water}[e]
ADI >= 5 mg/kg		R20, R21, R22, R36, R37, R38, R34, R35	a	A	B
ADI >= 0,1 mg/kg , < 5 mg/kg	R_F3, R_E3	R40/20, R40/21, R40/22, R23, R24, R25, R26, R27, R28, R39/23, R39/24, R39/25, R42, R64, R33, R48/20, R48/21, R48/22, R62, R63; carcinogenic but not persistent; default value	b	B	C
ADI < 0,1 mg/kg	C3 (MAK: IIIB), M3, R_F1, R_F2, R_E1, R_E2	R39/26, R39/27, R39/28, R43, R48, R48/23, R48/24, R48/25, R40, R60, R61	c	C	D
	C1 or C2 (MAK: IIIA1 or IIIA2), M1, M2	R45, R49, R46	d	D	E

[a] ADI: Acceptable daily intake per kg body weight and day
[b] R, 1,2, or 3: Embryo damaging; R, 1,2, or 3: Impairment of fertility; M 1,2, or 3: Mutagenicity (EU-commission)
[c] See **Table 1** for details
[d] Persistent or inherently degradable
[e] Accumulation as given by BCF > 100 or $\log P_{ow}$ > 3 as properties to be fulfilled

different classes. After that, a summation of the emitted amounts within each potential class is performed on the basis of mass units. Human toxicity does therefore not involve a characterization factor. A vertical aggregation over different toxicological potential classes to get a single equivalent load is not possible, because the effect intensity is not exactly quantifiable. This means the products can only be compared per potential class (→ *example Fig. 1*).

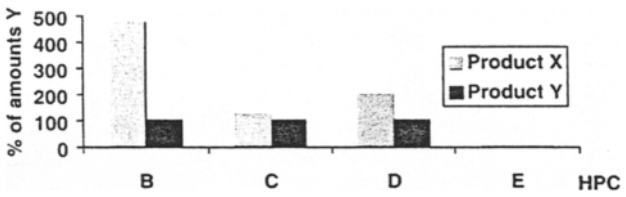

Fig. 1: Contributions of atmospheric (or waterborne) emissions to the impact category human toxicity for two assumed product alternatives X and Y. Only HPCs > "A" are considered which are of toxicological relevance. No emissions belonging to category E are found in our example. In the comparison between product X and Y the calculated effect scores can be displayed as a graph. The quantity of emitted substances within each HPC for product Y is arbitrarily settled to 100%

The product comparison is based both on the results of the here given "semi-quantitative screening method" and on toxicological expert knowledge. In the analysis step of the impact assessment, the results of the screening method (including the MACKAY-distributions) and the inventory data are weighed together with toxicological non-LCA data and scientific uncertainties to give a verbal summary and conclusion. Subjective judgement is excluded from this step as far as possible. The analysis should give the reasons for the preference of a particular product. One possible result of the analysis step might also be that there is not enough information for a product comparison in the effect category human toxicity. In this case it is necessary to include more information about space, frequency, and duration of emissions as well as some typical characteristics of the exposed areas (e.g. population density).

10 Discussion

Although the above described approach gives valuable information on hazard potentials from emissions, some limitations have to be taken into account.

The information on the emitted substances may be incomplete. For example, for metals often no distinction is made between the elemental and the ionic species. That is important for the reactivity and therefore for the behaviour in the organism. Moreover, specific substance mixtures are only registered as sum parameters (e.g. AOX, heavy metals, or VOC). Additionally only a limited amount of well-known substances are routinely measured and information on further critical emissions may be missing.

When considering exposure concentrations, not only the emitted amount is important but also the space into which a substance is emitted, the frequency and the duration of emissions. Additionally only those emissions are relevant, which lead to human exposure. For the evaluation it may be also of interest if the emission is into polluted or unpolluted areas. One way to deal with these problems is to characterise the site of an emission with a number of spatial aspects. The initial emitted amount of a critical stressor is then multi-

plied by an appropriate weighing factor (UDO DE HAES et al., 1995; KELLER et al., 1996; HERRCHEN et al., 1997b). For a start, the proposed method distinguishes between indoor and outdoor emissions. However this work is still in progress for evaluating toxic effects.

Concerning potential health effects, the proposed potential classes merely reflect the classified hazard potential of the emissions. The described method gives a good estimate of toxic effect-concentrations by using TLV-Values and R-Phrases but it gives no scientific sound statement as to the probable human risk because exposure concentrations are not available in LCA.

The separation into an inventory and effect assessment step results from formal aspects as well as from the sequential process of the LCA. However, the results are more relevant if already during the planning- and inventory-phase toxicological aspects are elaborated. For human health it may be sufficient to select the most relevant steps of a life cycle to compare products. This will reduce the work necessary and consequently the costs but will give much better results than former LCA, where toxicological aspects are considered only in the endphase.

11 Conclusions

A more differentiated statement that allows a quantitative product comparison is reserved to method Level 2 that is presently being developed by the Fraunhofer Institutes. Level 2 introduces a more detailed spatial differentiation of impacts by characterising and weighing emission sources through site-dependent exposure coefficients (KELLER et al., 1996). This implies, that then emissions in different amounts, at different times and at different places can be aggregated. To achieve this, more information is required for the evaluation at Level 2. An in-depth analysis of the exposure situations may not be possible for all life cycle steps. However certain steps, which can be assumed to give emissions of toxicological relevance, can be identified in advance. For these steps the following data must be collected:

- further specifications to spatial relationship,
- mode of exposure; whether continuous or intermittent,
- total duration and length of daily exposure,
- number of persons exposed (estimation).

The proposed method does **not** recommend a purely schematical procedure. Therefore, expert knowledge in the fields of single substance evaluation, toxicology, and exposure is needed during the analysis substep of the impact assessment.

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